The thermal neutron scattering measurements and analysis

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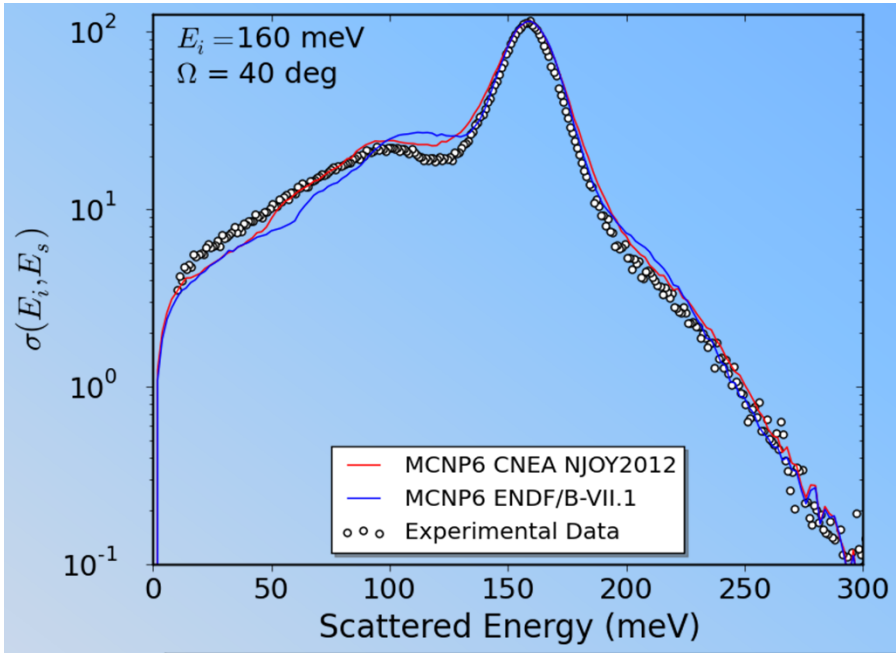
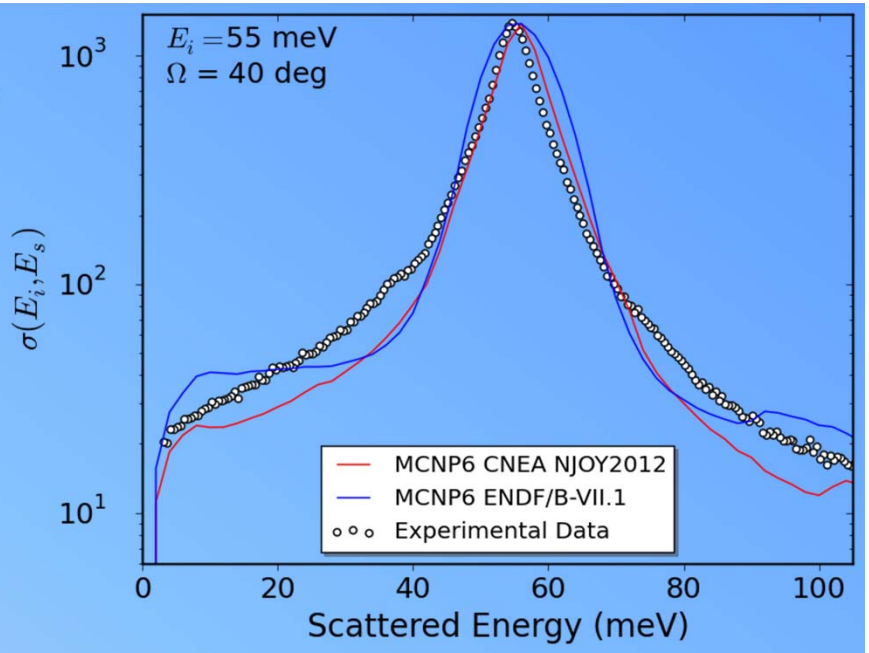
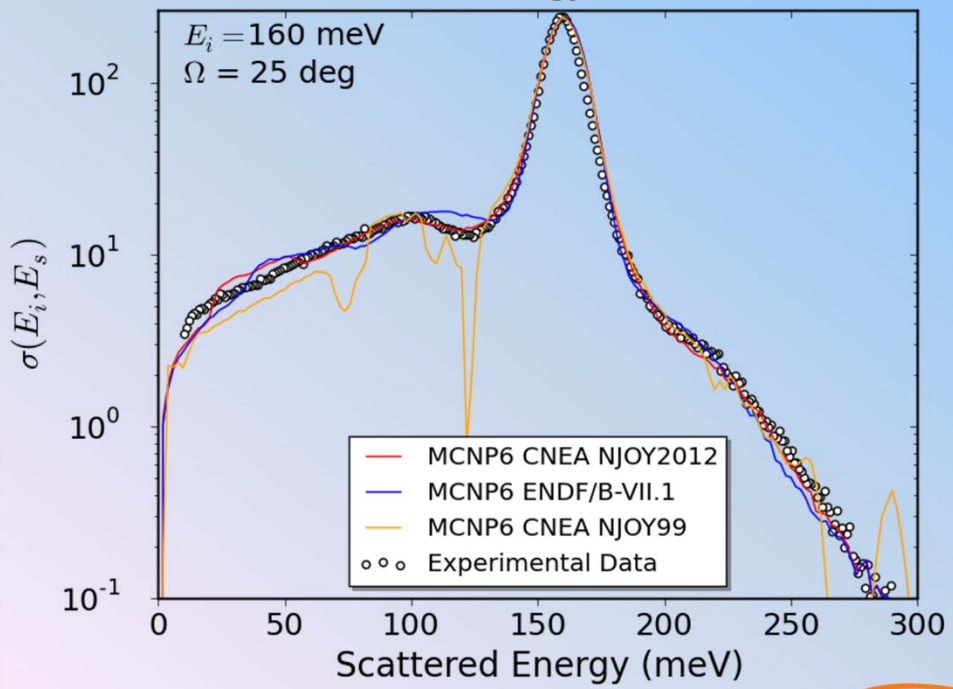
Thermal Scattering Overview

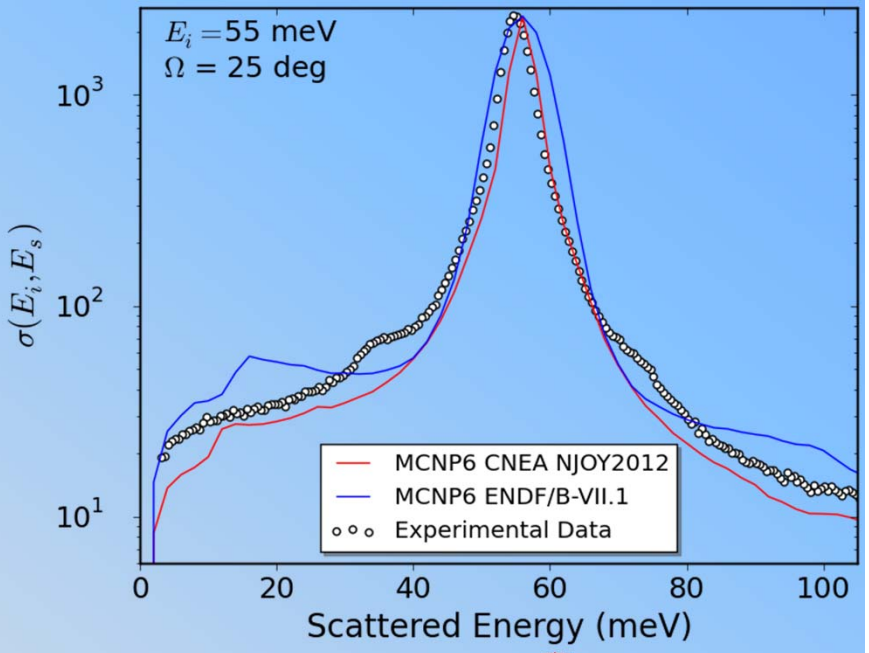
- Preformed measurements at SNS
  - SEQUOIA
    - Water
    - Medium Density Polyethylene (MDPE)
  - ARCS
    - High Density Polyethylene (HDPE) 295 K and 5 K
    - Quartz (SiO_2) at 20, 300, 550, 600 °C
  - VISION (measures $S(\omega)$)
    - Lucite, Lexan, Polyethylene at 5 K and 295 K
- The double differential scattering data (DDSD) can be used to benchmark thermal scattering evaluations
- Methods to generate $S(\alpha,\beta)$ from the experimental data are under development:
  1. Convert the data ($S(Q,\omega)$) to phonon spectrum (use low values of Q to limit multiple phonon scattering)
  2. Remove the elastic peak from the DDSD and convert the inelastic part directly to $S(\alpha,\beta)$
- Developed capabilities to use LAMMPS code to calculate the phonon spectrum and scattering kernel.

H_2O









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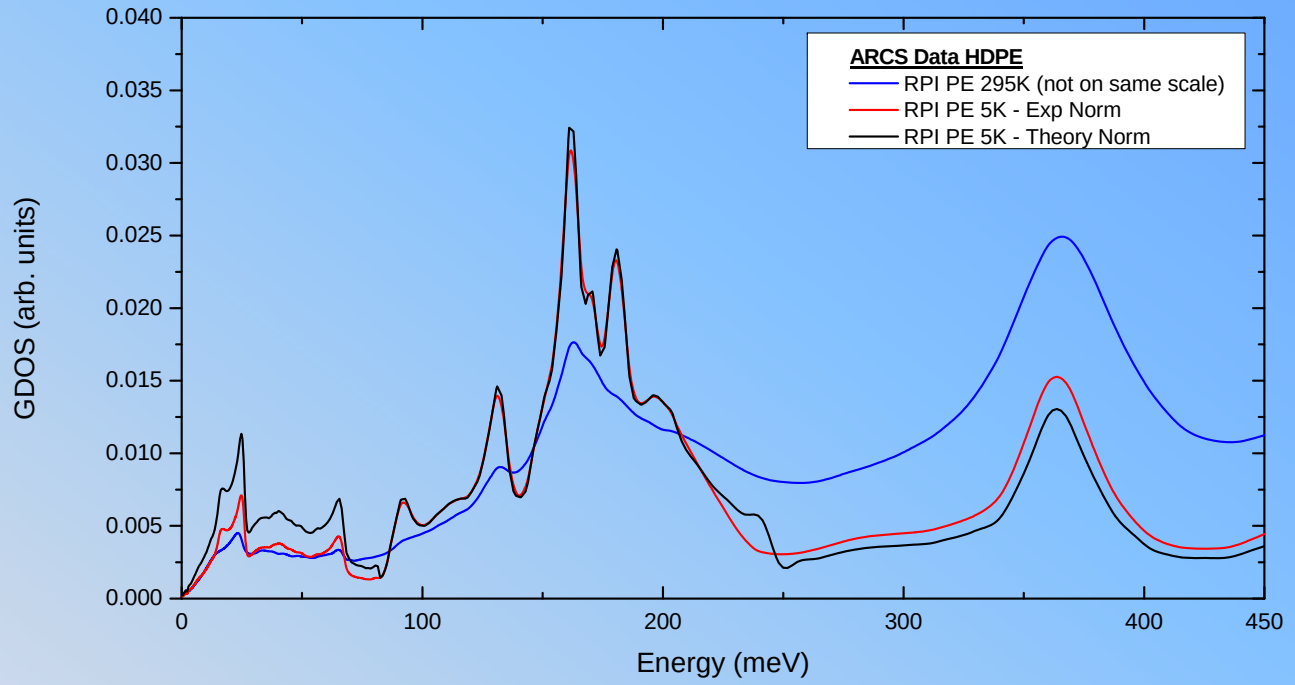
Phonon spectrum from measured $S(Q,E)$



- Low temperature measurements are essential in order to resolve the structure.
- Convert the measured $S(Q,E)$ data for phonon spectrum using the SNS DAVE code:

$$S(Q,E) = \frac{\hbar^2 Q^2}{6ME}\exp(-\langle u^2\rangle Q^2)G(E)[n(E,T)+1] \qquad n(E,T) = \frac{1}{\exp\left(\frac{E}{k_B T}\right)-1}$$

$G(E)$ - generalized phonon density-of-states(GDOS),
Q - wave vector transfer,
$S(Q,E)$ - structure dynamics factor,
M - mass of the atom,
$\langle u^2 \rangle$ - mean square displacement.

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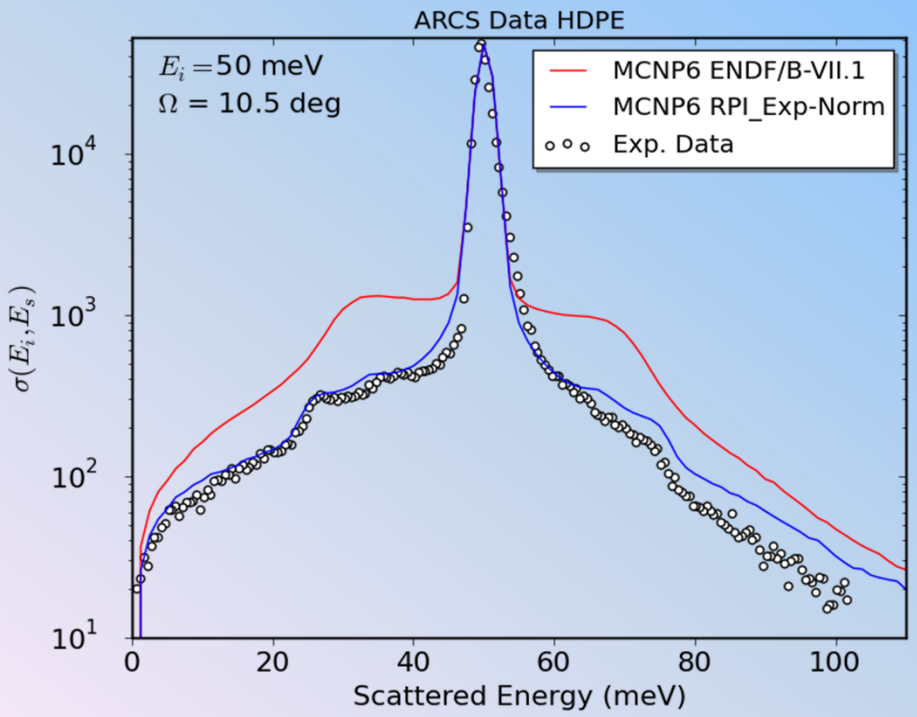
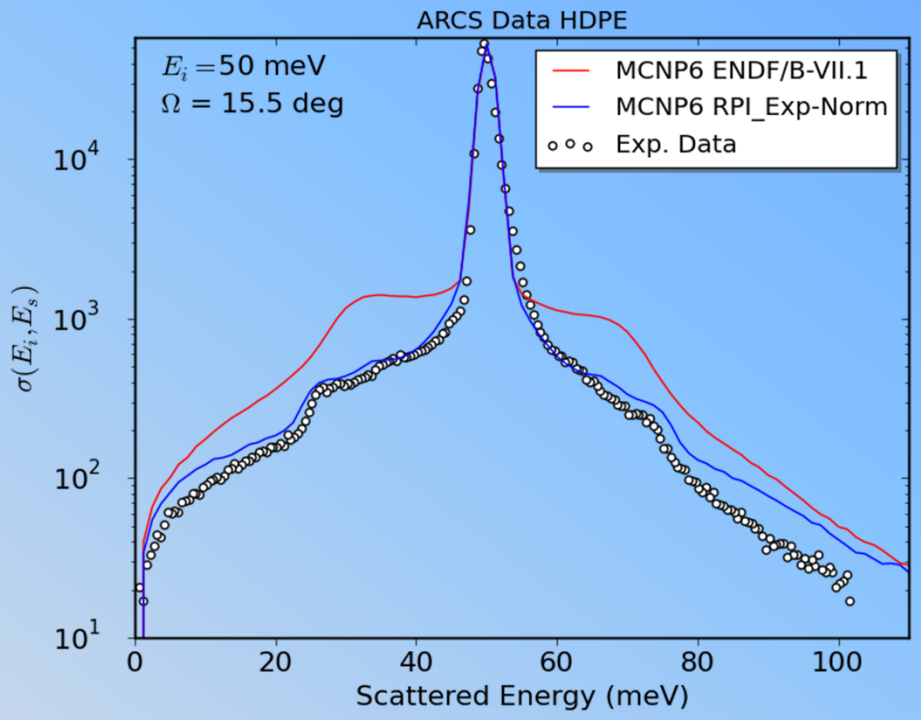
Example for HDPE

Experiment Normalized GDOS

- The phonon spectrum was processed with NJOY 2012
- The experimental response simulated with MCNP 6
- The agreement with the experiment is improved





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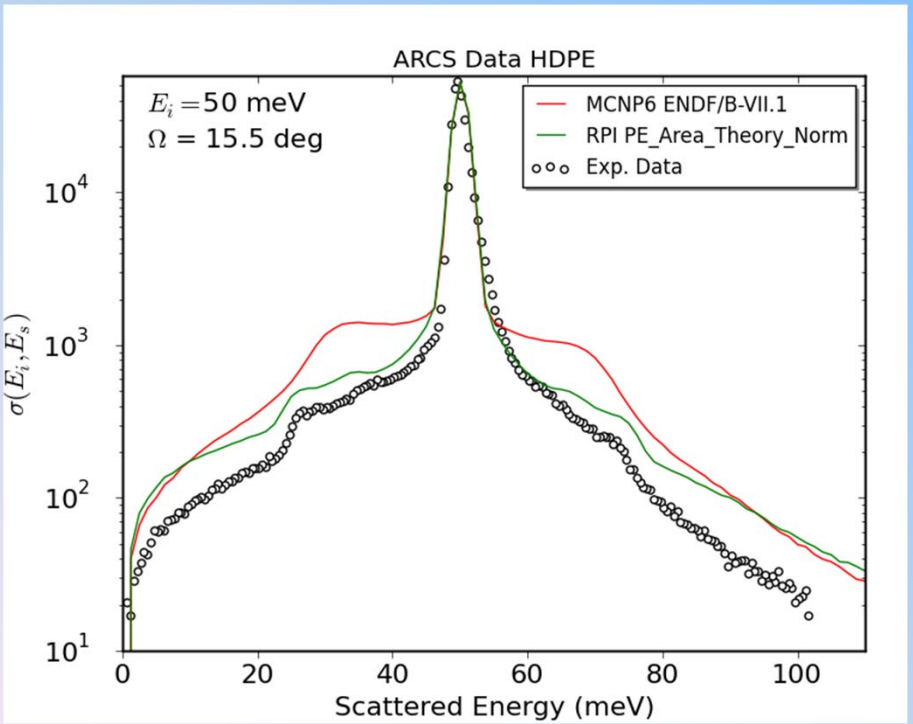
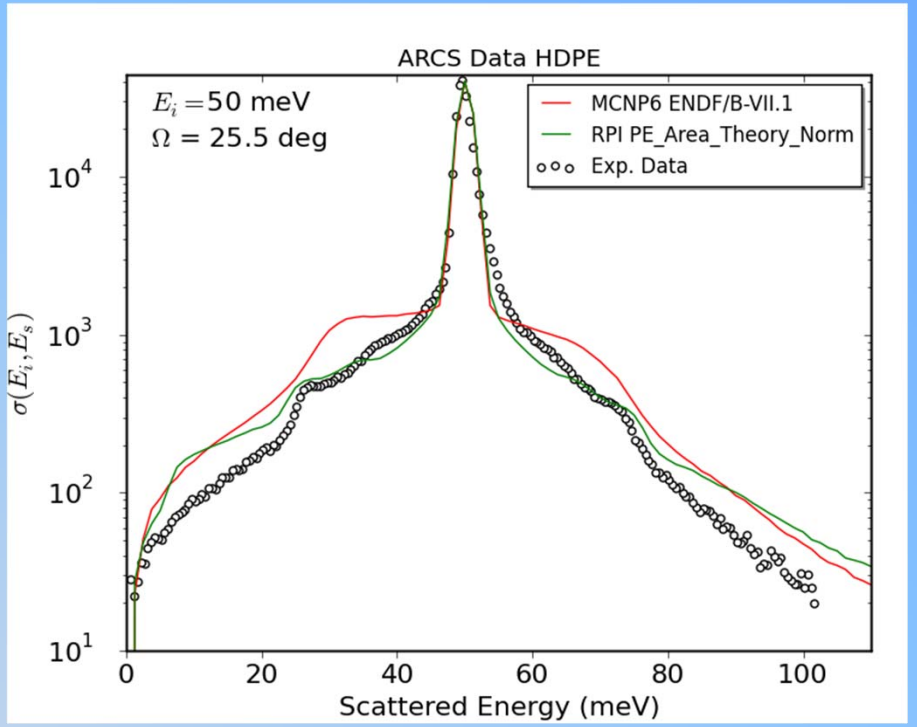
Example for HDPE
Theory Normalized GDOS

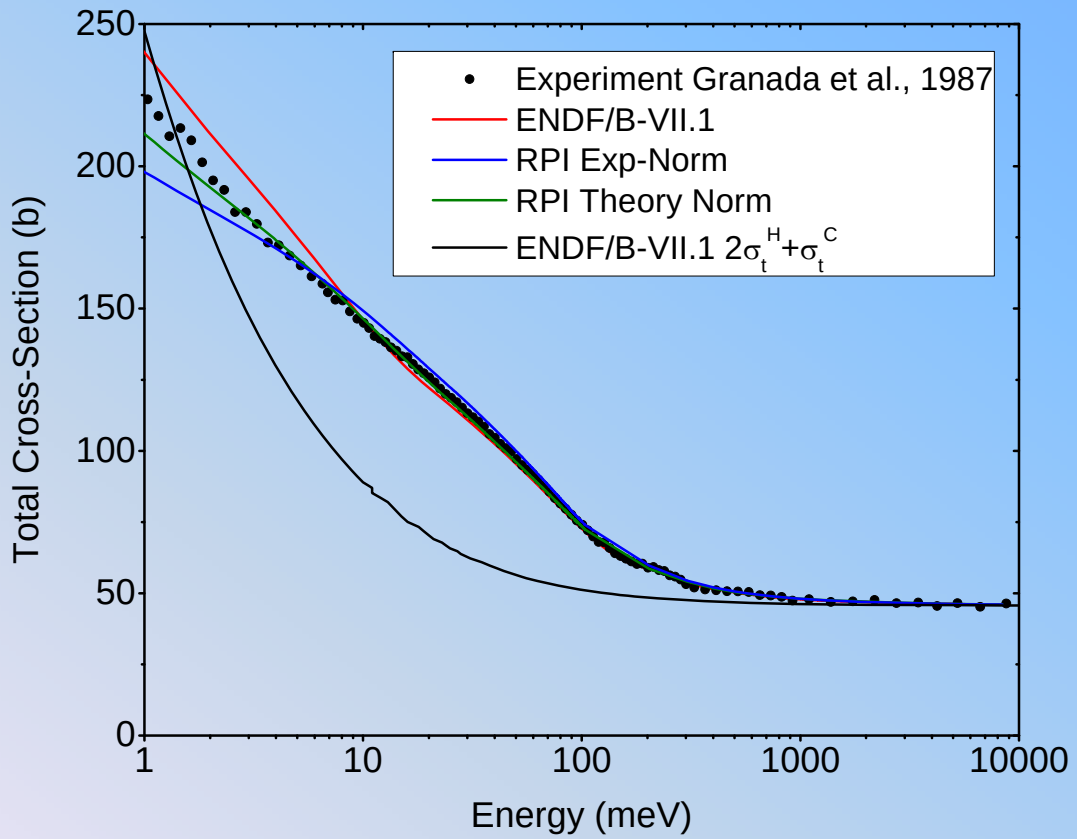
- Better agreement with total cross section but poorer agreement with double differential cross section.
- Other incident energies and angles available

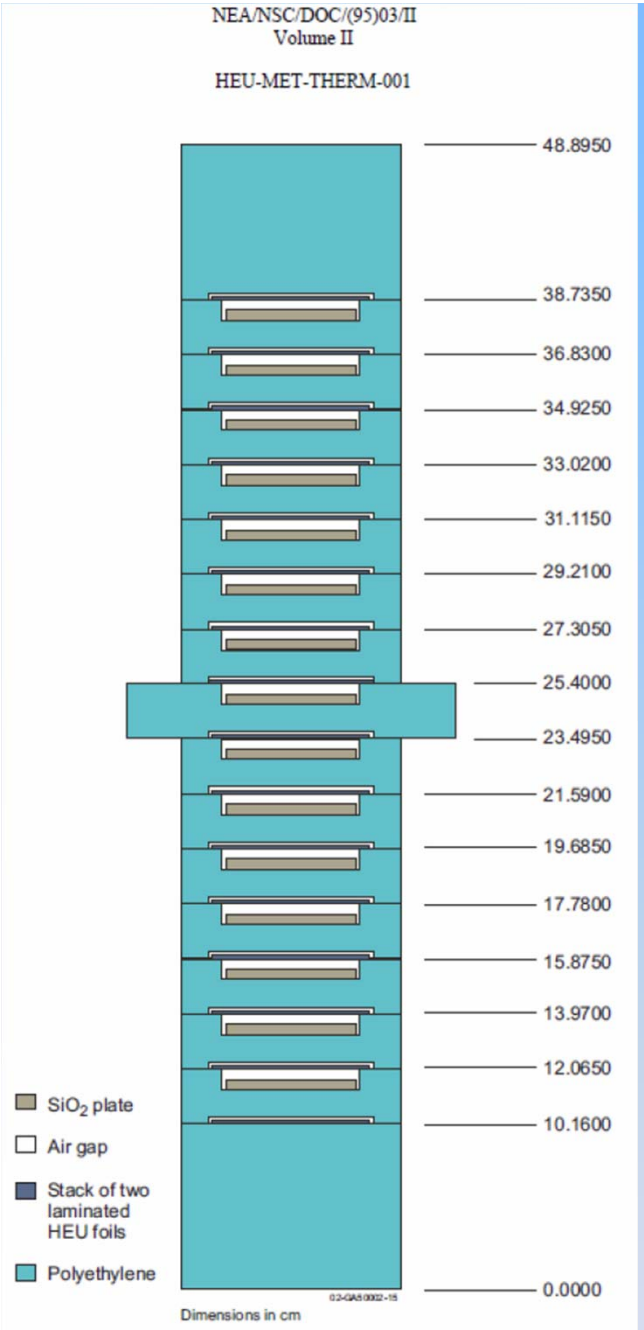




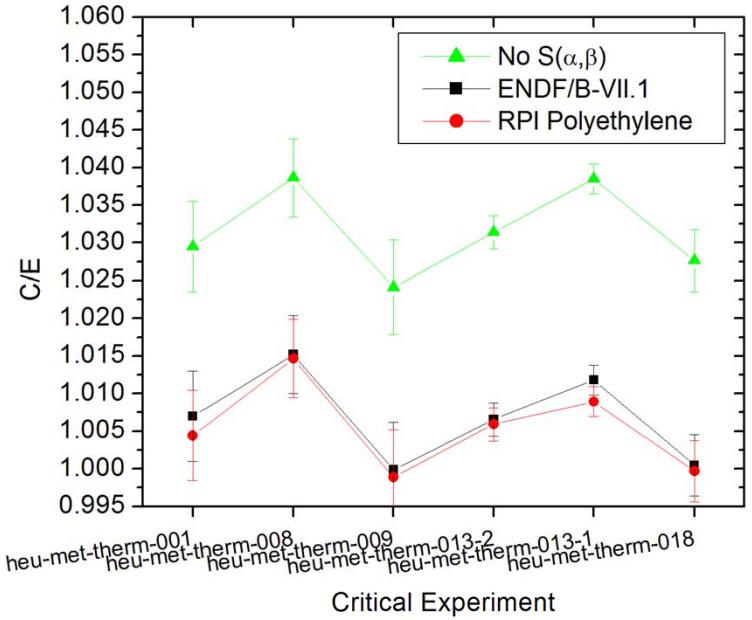
Polyethylene Total Cross Section

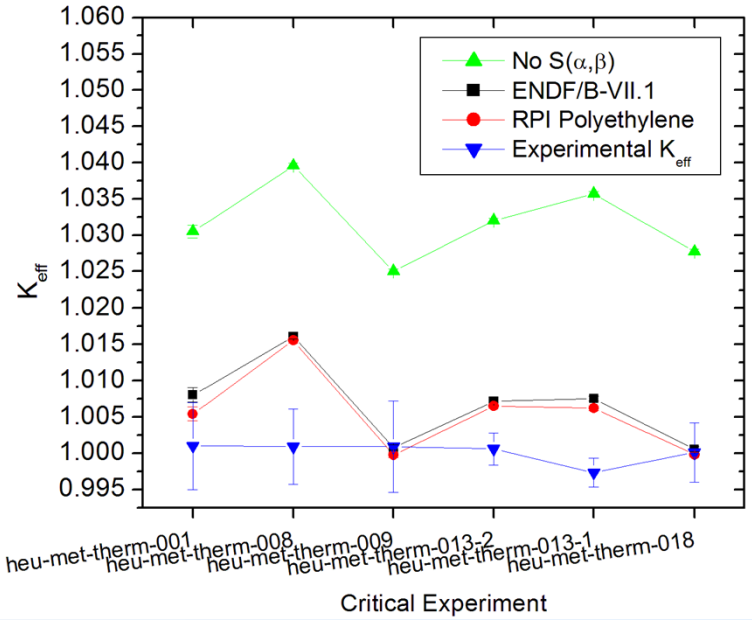
- The experimentally derived phonon spectrum is in good agreement with the total cross section measurement.
- Experimental vs theoretical normalization give slightly different results





Assemblies: Benchmark Model I





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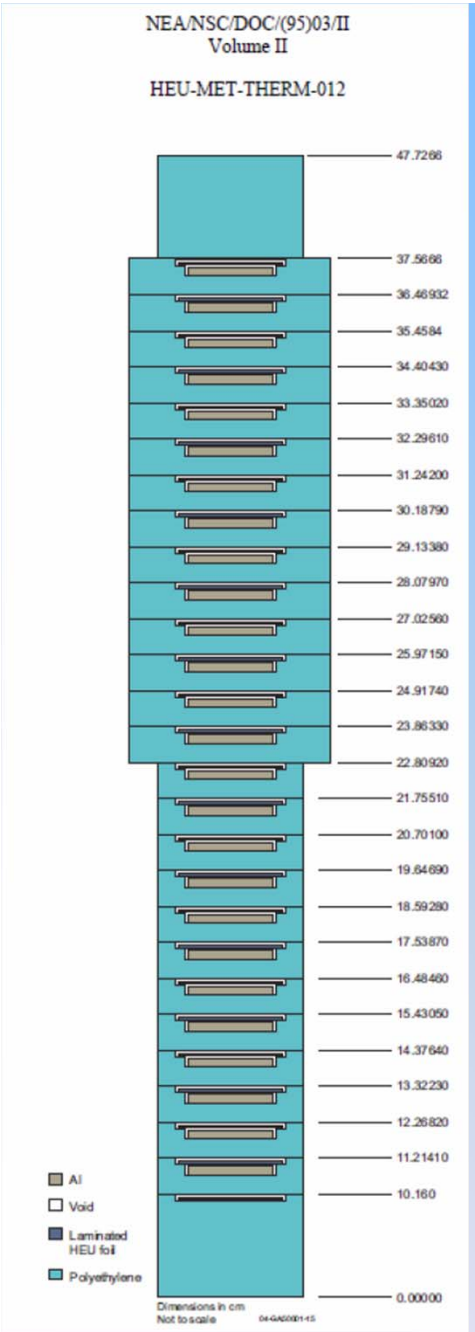
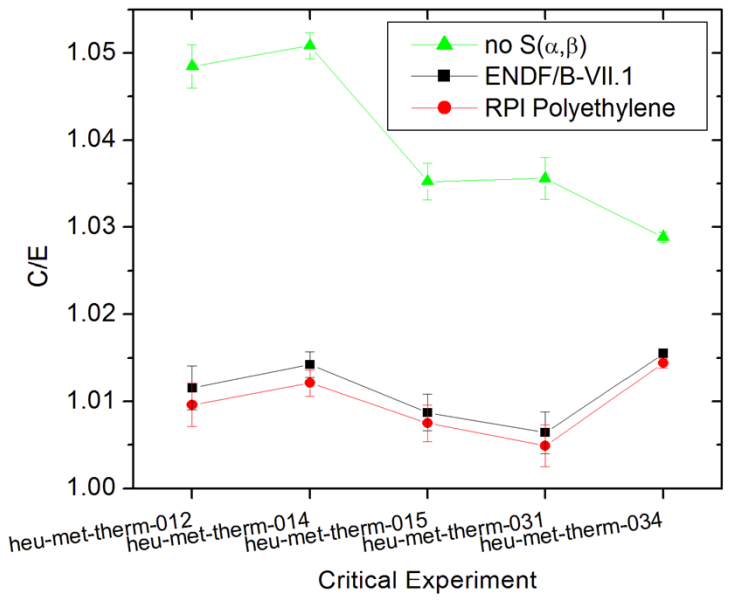
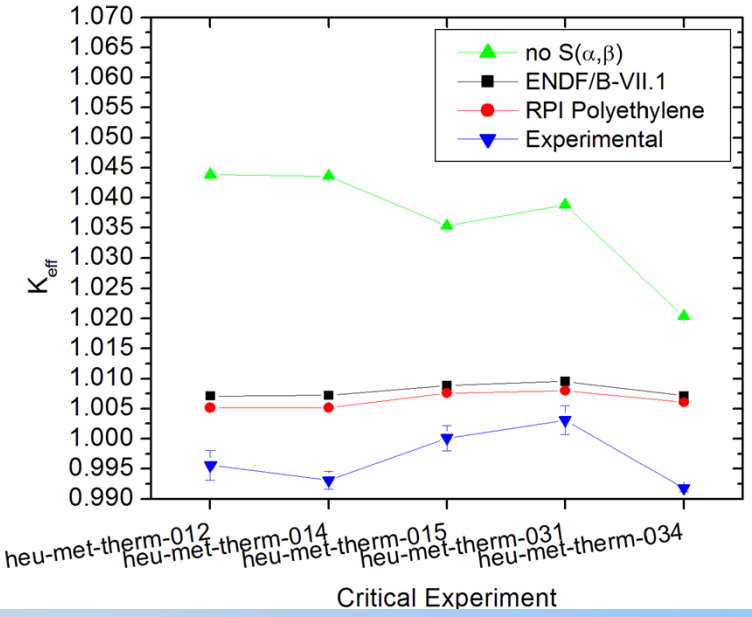


Assemblies: Benchmark Model II





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Questions?